Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.72e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.12e-01

Confidence level: 6.97e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Benzoquinone
Measured: 4.60e-12
Predicted: 5.97e-12

Image not found

1,3,5-Cycloheptatriene
Measured: 9.69e-11
Predicted: 1.00e-10